

AR201-13633 B

**SIDS Endpoints:****Review of Existing Data and Development of Test Plan Rational****1. GENERAL INFORMATION****[1.01 A.] CAS-number:** 109-72-8**[1.01 C.] Name of the Substance:** n-Butyllithium

Synonyms:

Lithium, butyl-

Butyllithium

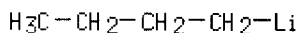
1-Butyllithium

Lithium, butyl- (8CI, 9CI) (CA INDEX NAME)

EINECS No.: 203-698-7

**[1.01 D.] CAS-descriptor:** Not applicable**[1.01 G.] Structural Formula**

The CAS file shows the following structure

**[1.5] Quantity**

Annual worldwide production and consumption of butyllithium and other organolithiums is 4 million pounds (1800 metric tonnes).<sup>1</sup>

**[1.7] Use Pattern**

Butyllithium reacts violently with air or water and is rarely used in its pure state. For safety and ease of use, butyllithium is diluted in hydrocarbon solvent and typical concentrations are 15-30% weight percent. Even when in a diluted state, butyllithium solutions are extremely reactive with air and are pyrophoric (spontaneously combustible). Butyllithium solutions are handled in sealed, inert gas systems and the utmost care taken to prevent environmental release or contamination from contact with air.

If butyllithium spills or otherwise comes in contact with ambient air, it decomposes almost immediately to form lithium hydroxide and butane. Precautions must be taken to prevent fire and prevent exposure to decomposed solutions, which are corrosive and flammable. Recommended cleanup measures minimize the possibility of exposure to skin or eyes. Recommended personal protection equipment for handling and spills includes chemical splash goggles with a face shield, rubber gloves, and rubber clothing.

Butyllithium is commonly used as an initiator for anionic polymerization in the manufacture of automobile tires. Some Butyllithium is used in organic synthesis to manufacture drugs and drug intermediates. It is handled in sealed systems under inert gas. Butyllithium is completely

<sup>1</sup> Weissenbacher, M., Anderson, E., Ishikawa, Y.; "Organometallics", July, 1998, page 681.7002T Chemical Economics Handbook-SRI International

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consumed in the manufacturing process and no residual amount is present in the end products. Butyllithium is not present in consumer products.

### [1.9] Sources of Exposure

Butyllithium is handled in closed systems under inert gas, and it is unlikely that exposure would occur. Sources of exposure would be limited to accidental spills, as might occur in an industrial process or in a transportation accident. Small releases would react immediately with air or moisture, forming butane and lithium hydroxide before it could come in contact with anyone in the surrounding area. Waste butyllithium would be chemically treated to hydrolyze it and neutralize the corrosive residue. Organic components of the waste would be burned for fuel. Human or environmental exposure is unlikely except in the case of an accident, in which case the resulting fire would consume the butyllithium. Accident response normally concentrates on controlling the effects of fire and heat on the surrounding area, and fires may be left to burn out on their own.

## 2. PHYSICAL-CHEMICAL DATA

### [2.3] Density (Relative Density)

**Densities of Commercially Available Butyllithium Solutions**

<b>n-Butyllithium formulation</b>	<b>density</b>	<b>Ref</b>
n-Butyllithium 24.0 % in Isopar C	0.707 g/ml (5.90 lb/gal) @ 20°C	FMC Lithium data sheet
n-Butyllithium 15 % in hexane	0.76 g/ml (6.34 lb/gal) @ 20°C	FMC Lithium data sheet
n-Butyllithium 25.0 wt. % in heptanes	0.72 g/ml (6.01 lb/gal)	FMC Lithium data sheet
n-Butyllithium 24% in heptane	0.697 g/cc	1. Kamienski; Esmay, J.Org.Chem., 25 1960, 115,119,120, CODEN: JOCEAH

The following physical property information is not available, and it is not practical to run the studies according to given protocols because butyllithium and butyllithium solutions are pyrophoric. Any study procedure that does not exclude air and moisture would not produce meaningful data and is of no value.

#### [2.1] Melting Point <sup>2</sup>

#### [2.2] Boiling Point

#### [2.4] Vapour Pressure

#### [2.5] Partition Coefficient (n-Octanol/water)

#### [2.6. A.] Water Solubility

#### [2.6.B.] pH Value and pKa Value

#### [2.12] Oxidation-Reduction Potential

#### [2.13 A.] Adsorption/ Desorption to Soil

<sup>2</sup> The melting point of Butyllithium is less than 0 °C. Pure butyllithium is a liquid. In commercial formulations the solvent properties control the melting point.)

### 3. ENVIRONMENTAL FATE AND PATHWAYS

The following environmental studies cannot be conducted on butyllithium because it is pyrophoric. Any study procedure that does not exclude air and moisture would not produce meaningful data and is of no value. Butyllithium reacts violently with water to form butane and lithium hydroxide. Butane is a HPV chemical already supported by the American Petroleum Institute (API) Petroleum HPV Testing Group, and American Chemistry Council (ACC) Olefins Panel HPV Work Group.<sup>3</sup> Lithium hydroxide may raise the pH of aquatic systems.

#### [3.1.1] Photodegradation

#### [3.1.2] Stability in Water (Hydrolysis)

#### [3.2] Monitoring Data (Environment)

#### [3.3] Transport and Distribution between Environmental Compartments including Estimated Environmental Concentrations and Distribution Pathways

#### [3.5] Biodegradation

### 4. ECOTOXICITY, and 5. TOXICITY

Studies to determine the ecotoxicity and animal toxicity cannot be performed on butyllithium because of its reactivity and corrosive properties. Butyllithium is pyrophoric and would react violently on exposure to aquatic systems and animal tissues, releasing flammable butane and corrosive lithium hydroxide, and likely starting a fire. Exposure of butyllithium to test animals would be cruel and not generate meaningful data as the test animals would most likely have to be sacrificed for humane reasons long before the study concluded. In fact, the use of any test method where water and air is not excluded is of no value.

Experiences with human exposure (item 5.11 of the SIDS data set) can be provided, and is included below.

#### 4. ECOTOXICITY

##### [4.1] Acute/Prolonged Toxicity to Fish

##### [4.2.A] Acute Toxicity to Aquatic Invertebrates (Daphnia)

##### [4.3] Toxicity to Aquatic plants e.g. Algae

##### [4.5.2] Chronic Toxicity to Aquatic Invertebrates (Daphnia)

##### [4.6] Toxicity to Terrestrial Organisms

#### 5. TOXICITY

##### [5.1] Acute Toxicity

##### [5.4] Repeated dose Toxicity

##### [5.5] [5.6] Genetic Toxicity in vitro and in vivo

##### [5.7] Toxicity to Reproduction

##### [5.8] Developmental Toxicity/Teratogenicity

#### [5.11] Experiences with Human Exposure (Work Place Exposure)

Butyllithium is used in closed systems under an inert atmosphere and human exposure is rare.

<sup>3</sup> See entry under butane, CAS No. 106978, on the EPA website address: <http://www.epa.gov/oppt/chemrtk/opptsrch.htm>.

No concentrations of butyllithium would be present in the work place because it reacts immediately with air or ambient moisture to form butane and lithium hydroxide. It is consumed completely in the industrial manufacturing processes in which it is used and is not present in the final product. Therefore, there is no exposure from use of final product.

In cases where workers might be exposed to butyllithium or decomposed butyllithium solutions, the MSDS recommends splash goggles with a face shield, rubber gloves, and rubber clothing.